

2,2-Diphenyl-4-(piperidin-1-yl)-butanamide

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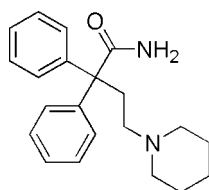
Received 20 June 2011; accepted 22 June 2011

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}—\text{C}) = 0.002$ Å; R factor = 0.036; wR factor = 0.102; data-to-parameter ratio = 21.5.

In the title compound, $\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}$, the dihedral angle between the mean planes of the two benzene rings is 81.1 (9)°. The piperidine ring is in a chair conformation. The crystal packing is stabilized by $\text{N}—\text{H} \cdots \text{N}$ and $\text{N}—\text{H} \cdots \text{O}$ hydrogen bonds and weak intermolecular $\text{C}—\text{H} \cdots \text{O}$ interactions.

Related literature

For the biological activity and pharmaceutical applications of compounds similar to the title compound, see: Guzel *et al.* (2006). For related structures, see: Akkurt *et al.* (2007); Dutkiewicz *et al.* (2010); Gerkin (1998); Krigbaum *et al.* (1968); Narasegowda *et al.* (2005); Yathirajan *et al.* (2005). For standard bond lengths, see Allen *et al.* (1987). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{26}\text{N}_2\text{O}$ $V = 1793.7$ (2) Å³
 $M_r = 322.44$ $Z = 4$
Orthorhombic, $Pca2_1$ Mo $K\alpha$ radiation
 $a = 18.1070$ (12) Å $\mu = 0.07$ mm⁻¹
 $b = 10.3025$ (9) Å $T = 173$ K
 $c = 9.6150$ (6) Å $0.40 \times 0.32 \times 0.20$ mm

Data collection

Oxford Diffraction Xcalibur Eos 19279 measured reflections
Gemini diffractometer 4817 independent reflections
Absorption correction: multi-scan 4547 reflections with $I > 2\sigma(I)$
(*CrysAlis RED*; Oxford $R_{\text{int}} = 0.020$
Diffraction, 2010)
 $T_{\text{min}} = 0.971$, $T_{\text{max}} = 0.986$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$ H atoms treated by a mixture of
 $wR(F^2) = 0.102$ independent and constrained
 $S = 1.02$ refinement
4817 reflections $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
224 parameters $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³
4 restraints

Table 1

Hydrogen-bond geometry (Å, °).

| $D—H \cdots A$ | $D—H$ | $H \cdots A$ | $D \cdots A$ | $D—H \cdots A$ |
|--|----------|--------------|--------------|----------------|
| $\text{N1}—\text{H1NB} \cdots \text{N2}^{\text{i}}$ | 0.87 (1) | 2.08 (1) | 2.9457 (13) | 177 (2) |
| $\text{N1}—\text{H1NA} \cdots \text{O1}^{\text{ii}}$ | 0.84 (1) | 2.38 (1) | 3.1971 (14) | 164 (2) |
| $\text{C3}—\text{H3B} \cdots \text{O1}^{\text{ii}}$ | 0.99 | 2.47 | 3.3738 (14) | 152 |

Symmetry codes: (i) $-x + \frac{3}{2}, y, z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, y, z - \frac{1}{2}$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

MSS thanks the University of Mysore for research facilities and HSY thanks R. L. Fine Chem, Bangalore, India, for the gift sample. JPJ acknowledges the NSF–MRI program (grant No. CHE1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5167).

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supporting information

Acta Cryst. (2011). E67, o1827 [doi:10.1107/S1600536811024585]

2,2-Diphenyl-4-(piperidin-1-yl)butanamide

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S1. Comment

The title compound is an intermediate used in the synthesis of biologically and pharmaceutically active compounds viz., loperamide, darifenacin, fempiverine, etc. The synthesis and antimycobacterial activity of some new related 2,2-diphenylacetamide derivatives has been described (Guzel *et al.*, 2006). The crystal structures of N,N-diphenylacetamide (Krigbaum *et al.*, 1968), 4,4'-dimethylbiphenyl-2,2'-dicarboxylic acid (Gerkin, 1998), 4'-methylbiphenyl-2-carboxylic acid (Narasegowda *et al.*, 2005) and 4'-(2-butyl-4-chloro-5-formylimidazol-1-ylmethyl) biphenyl-2-carbonitrile (Yathirajan *et al.*, 2005), 2-hydroxy-N-(3-oxo-1-thia-4-azaspiro[4.5]dec-4-yl)-2,2-diphenylacetamide (Akkurt *et al.*, 2007) and 2-chloro-N-[4-chloro-2-(2-chlorobenzoyl) phenyl]acetamide (Dutkiewicz *et al.*, 2010) have been reported. In view of the importance of the title compound, (I), $C_{21}H_{26}N_2O$, a new crystal structure determination is reported.

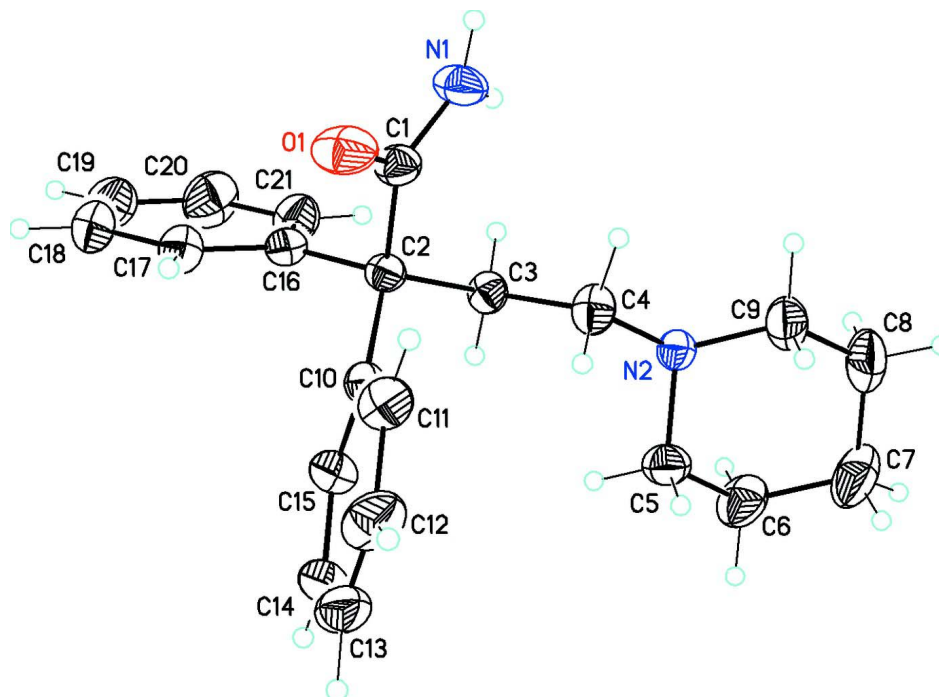
In the title compound, (I), the dihedral angle between the mean planes of the two benzene rings is $81.1(9)^\circ$ (Fig. 1). The piperidin-1-yl ring is in a chair conformation (Cremer & Pople (1975), puckering parameters Q , θ , and $\varphi = 0.5689(15)\text{\AA}$, $3.89(16)^\circ$ and $14(2)^\circ$ respectively). For an ideal chair θ has a value of 0 or 180° . Bond lengths are normal (Allen *et al.*, 1987). Crystal packing is stabilized by N—H \cdots N, N—H \cdots O hydrogen bonds and weak C—H \cdots O intermolecular interactions (Fig. 2, Table 1).

S2. Experimental

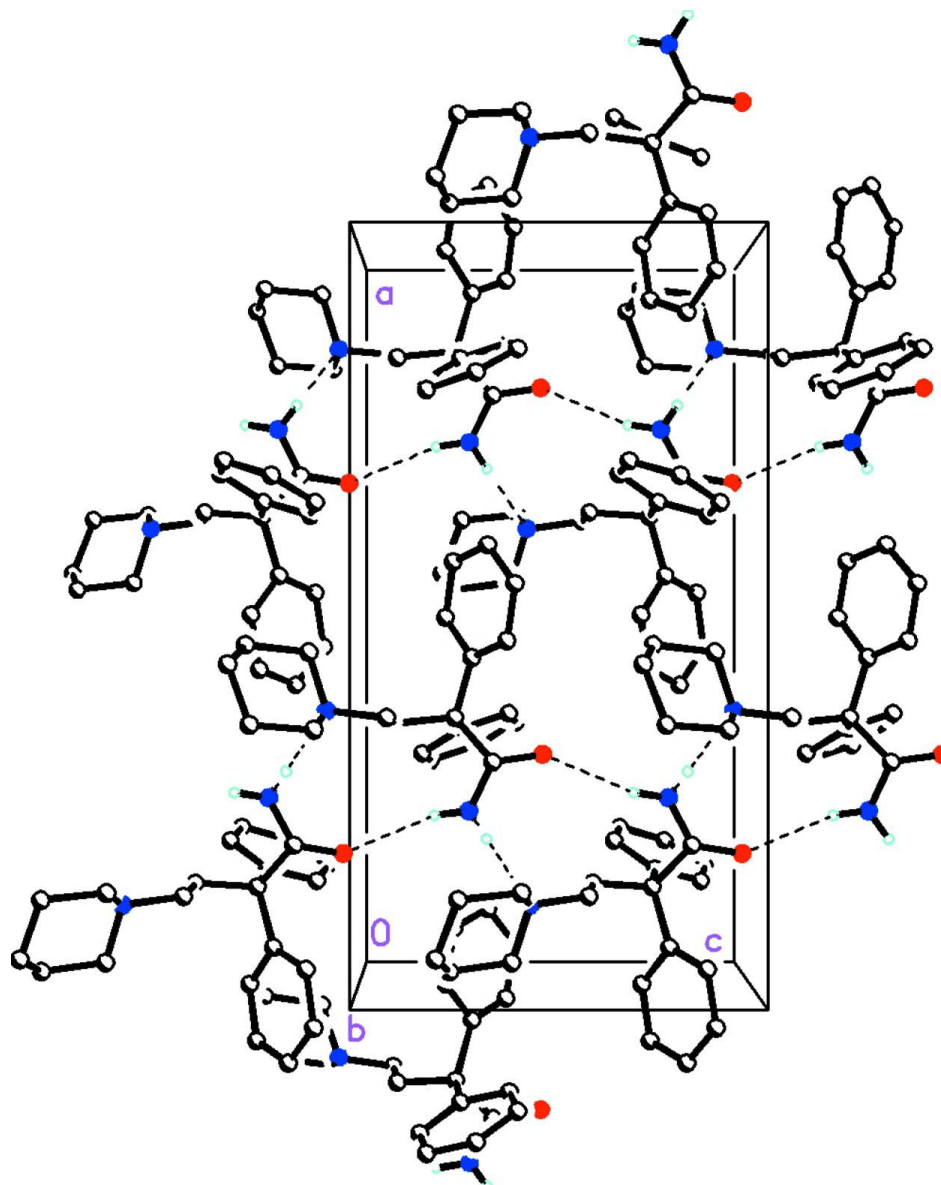
The title compound was obtained as a gift sample from R. L. Fine Chem, Bangalore. X-ray quality crystals were obtained by slow evaporation of (1:1) methanol and dichloromethane solution (m.p.: 458-460 K).

S3. Refinement

The N—H atoms were located by Fourier analysis and refined isotropically with $DFIX = 0.86\text{\AA}$ and $DANG = 1.40\text{\AA}$. All of the remaining H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.95\AA (CH), or 0.99\AA (CH_2). Isotropic displacement parameters for these atoms were set to 1.18-1.20 (CH) or (CH_2) times U_{eq} of the parent atom.

**Figure 1**

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

**Figure 2**

Packing diagram of the title compound viewed down the *b* axis. Dashed lines represent N—H...N, N—H...O hydrogen bonds and weak C—H...O intermolecular interactions.

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Crystal data

$C_{21}H_{26}N_2O$
 $M_r = 322.44$
 Orthorhombic, $Pca2_1$
 Hall symbol: $P\ 2c\ -2ac$
 $a = 18.1070\ (12)\ \text{\AA}$
 $b = 10.3025\ (9)\ \text{\AA}$
 $c = 9.6150\ (6)\ \text{\AA}$
 $V = 1793.7\ (2)\ \text{\AA}^3$
 $Z = 4$

$F(000) = 696$
 $D_x = 1.194\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$
 Cell parameters from 9220 reflections
 $\theta = 3.4\text{--}32.5^\circ$
 $\mu = 0.07\ \text{mm}^{-1}$
 $T = 173\ \text{K}$
 Block, colorless
 $0.40 \times 0.32 \times 0.20\ \text{mm}$

Data collection

Oxford Diffraction Xcalibur Eos Gemini
diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1500 pixels mm⁻¹
 ω scans
Absorption correction: multi-scan
(*CrysAlis RED*; Oxford Diffraction, 2010)
 $T_{\min} = 0.971$, $T_{\max} = 0.986$

19279 measured reflections
4817 independent reflections
4547 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 $\theta_{\max} = 29.1^\circ$, $\theta_{\min} = 3.7^\circ$
 $h = -24 \rightarrow 24$
 $k = -13 \rightarrow 14$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.102$
 $S = 1.02$
4817 reflections
224 parameters
4 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.1453P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.16 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|--------------|--------------|----------------------------------|
| O1 | 0.68400 (5) | 0.34583 (11) | 0.96707 (9) | 0.0432 (2) |
| N1 | 0.75885 (6) | 0.33139 (12) | 0.78130 (11) | 0.0375 (2) |
| H1NB | 0.7944 (8) | 0.2941 (16) | 0.8267 (16) | 0.045* |
| H1NA | 0.7651 (9) | 0.3416 (16) | 0.6956 (14) | 0.045* |
| N2 | 0.62349 (5) | 0.19366 (9) | 0.43291 (9) | 0.02659 (18) |
| C1 | 0.69459 (6) | 0.36080 (11) | 0.84208 (11) | 0.0287 (2) |
| C2 | 0.63630 (5) | 0.42567 (10) | 0.74607 (9) | 0.02408 (18) |
| C3 | 0.64319 (6) | 0.37719 (10) | 0.59391 (10) | 0.02621 (19) |
| H3A | 0.6058 | 0.4219 | 0.5361 | 0.031* |
| H3B | 0.6925 | 0.4011 | 0.5577 | 0.031* |
| C4 | 0.63287 (7) | 0.23102 (11) | 0.57931 (11) | 0.0318 (2) |
| H4A | 0.6764 | 0.1858 | 0.6183 | 0.038* |
| H4B | 0.5889 | 0.2036 | 0.6330 | 0.038* |
| C5 | 0.54694 (6) | 0.21203 (12) | 0.38868 (13) | 0.0356 (2) |
| H5A | 0.5320 | 0.3030 | 0.4065 | 0.043* |

| | | | | |
|------|--------------|--------------|--------------|------------|
| H5B | 0.5144 | 0.1547 | 0.4440 | 0.043* |
| C6 | 0.53738 (9) | 0.18176 (15) | 0.23557 (15) | 0.0470 (3) |
| H6A | 0.5671 | 0.2433 | 0.1797 | 0.056* |
| H6B | 0.4849 | 0.1928 | 0.2094 | 0.056* |
| C7 | 0.56157 (11) | 0.04385 (16) | 0.20378 (18) | 0.0579 (4) |
| H7A | 0.5270 | −0.0182 | 0.2477 | 0.070* |
| H7B | 0.5606 | 0.0292 | 0.1020 | 0.070* |
| C8 | 0.63853 (10) | 0.02107 (16) | 0.25826 (18) | 0.0578 (4) |
| H8A | 0.6740 | 0.0726 | 0.2028 | 0.069* |
| H8B | 0.6513 | −0.0718 | 0.2471 | 0.069* |
| C9 | 0.64546 (8) | 0.05852 (13) | 0.41083 (16) | 0.0438 (3) |
| H9A | 0.6138 | 0.0009 | 0.4677 | 0.053* |
| H9B | 0.6972 | 0.0465 | 0.4414 | 0.053* |
| C10 | 0.55575 (5) | 0.40102 (11) | 0.78870 (11) | 0.0274 (2) |
| C11 | 0.53249 (7) | 0.30304 (12) | 0.87673 (13) | 0.0371 (2) |
| H11A | 0.5678 | 0.2506 | 0.9235 | 0.044* |
| C12 | 0.45683 (8) | 0.28120 (16) | 0.89694 (16) | 0.0494 (3) |
| H12A | 0.4414 | 0.2148 | 0.9589 | 0.059* |
| C13 | 0.40475 (7) | 0.35405 (17) | 0.82879 (16) | 0.0498 (4) |
| H13A | 0.3537 | 0.3367 | 0.8417 | 0.060* |
| C14 | 0.42691 (7) | 0.45219 (15) | 0.74177 (16) | 0.0455 (3) |
| H14A | 0.3912 | 0.5038 | 0.6951 | 0.055* |
| C15 | 0.50184 (6) | 0.47598 (12) | 0.72201 (13) | 0.0361 (2) |
| H15A | 0.5167 | 0.5445 | 0.6621 | 0.043* |
| C16 | 0.65362 (5) | 0.57150 (11) | 0.76043 (11) | 0.0287 (2) |
| C17 | 0.63429 (7) | 0.63353 (13) | 0.88404 (14) | 0.0404 (3) |
| H17A | 0.6108 | 0.5856 | 0.9559 | 0.048* |
| C18 | 0.64896 (8) | 0.76405 (15) | 0.90339 (19) | 0.0528 (4) |
| H18A | 0.6355 | 0.8050 | 0.9882 | 0.063* |
| C19 | 0.68294 (9) | 0.83480 (15) | 0.8005 (2) | 0.0565 (4) |
| H19A | 0.6922 | 0.9248 | 0.8133 | 0.068* |
| C20 | 0.70346 (9) | 0.77430 (15) | 0.6784 (2) | 0.0544 (4) |
| H20A | 0.7272 | 0.8228 | 0.6073 | 0.065* |
| C21 | 0.68962 (7) | 0.64287 (13) | 0.65859 (15) | 0.0400 (3) |
| H21A | 0.7049 | 0.6018 | 0.5749 | 0.048* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|------------|------------|------------|-------------|-------------|-------------|
| O1 | 0.0344 (4) | 0.0706 (6) | 0.0246 (4) | 0.0036 (4) | −0.0032 (3) | 0.0074 (4) |
| N1 | 0.0269 (4) | 0.0567 (6) | 0.0288 (5) | 0.0099 (4) | −0.0038 (4) | −0.0007 (4) |
| N2 | 0.0269 (4) | 0.0282 (4) | 0.0246 (4) | 0.0000 (3) | −0.0001 (3) | −0.0028 (3) |
| C1 | 0.0264 (5) | 0.0341 (5) | 0.0256 (5) | 0.0012 (4) | −0.0037 (4) | 0.0008 (4) |
| C2 | 0.0227 (4) | 0.0304 (5) | 0.0191 (4) | 0.0022 (3) | −0.0005 (3) | −0.0003 (3) |
| C3 | 0.0299 (5) | 0.0296 (5) | 0.0192 (4) | 0.0006 (4) | 0.0005 (3) | −0.0002 (4) |
| C4 | 0.0431 (6) | 0.0296 (5) | 0.0228 (5) | 0.0013 (4) | −0.0025 (4) | 0.0018 (4) |
| C5 | 0.0285 (5) | 0.0430 (6) | 0.0352 (6) | 0.0008 (4) | −0.0033 (4) | −0.0015 (5) |
| C6 | 0.0552 (8) | 0.0479 (7) | 0.0380 (6) | −0.0021 (6) | −0.0164 (6) | −0.0029 (6) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C7 | 0.0775 (11) | 0.0478 (8) | 0.0485 (8) | −0.0076 (7) | −0.0186 (7) | −0.0154 (6) |
| C8 | 0.0703 (10) | 0.0462 (8) | 0.0569 (9) | 0.0083 (7) | −0.0041 (8) | −0.0266 (7) |
| C9 | 0.0501 (7) | 0.0324 (6) | 0.0490 (7) | 0.0079 (5) | −0.0094 (6) | −0.0099 (5) |
| C10 | 0.0248 (4) | 0.0335 (5) | 0.0239 (4) | −0.0001 (4) | 0.0009 (4) | −0.0062 (4) |
| C11 | 0.0374 (6) | 0.0427 (6) | 0.0311 (6) | −0.0058 (5) | 0.0018 (4) | 0.0010 (5) |
| C12 | 0.0445 (7) | 0.0618 (8) | 0.0419 (7) | −0.0220 (6) | 0.0100 (5) | −0.0038 (6) |
| C13 | 0.0299 (6) | 0.0715 (10) | 0.0480 (7) | −0.0109 (6) | 0.0058 (5) | −0.0213 (7) |
| C14 | 0.0272 (5) | 0.0587 (8) | 0.0506 (7) | 0.0074 (5) | −0.0032 (5) | −0.0175 (6) |
| C15 | 0.0285 (5) | 0.0397 (6) | 0.0402 (6) | 0.0047 (4) | −0.0014 (4) | −0.0032 (5) |
| C16 | 0.0245 (4) | 0.0322 (5) | 0.0293 (5) | 0.0009 (4) | −0.0038 (4) | −0.0028 (4) |
| C17 | 0.0371 (6) | 0.0442 (7) | 0.0399 (7) | −0.0008 (5) | 0.0004 (5) | −0.0117 (5) |
| C18 | 0.0443 (7) | 0.0509 (8) | 0.0632 (9) | 0.0003 (6) | −0.0042 (6) | −0.0278 (7) |
| C19 | 0.0467 (8) | 0.0382 (7) | 0.0846 (12) | −0.0066 (6) | −0.0075 (8) | −0.0158 (7) |
| C20 | 0.0576 (9) | 0.0411 (7) | 0.0646 (10) | −0.0136 (6) | −0.0005 (7) | 0.0018 (6) |
| C21 | 0.0440 (6) | 0.0380 (6) | 0.0379 (6) | −0.0065 (5) | 0.0011 (5) | −0.0018 (5) |

Geometric parameters (Å, °)

| | | | |
|--------------|-------------|-----------|-------------|
| O1—C1 | 1.2267 (14) | C8—H8A | 0.9900 |
| N1—C1 | 1.3368 (14) | C8—H8B | 0.9900 |
| N1—H1NB | 0.867 (12) | C9—H9A | 0.9900 |
| N1—H1NA | 0.838 (13) | C9—H9B | 0.9900 |
| N2—C5 | 1.4621 (14) | C10—C11 | 1.3830 (16) |
| N2—C9 | 1.4635 (14) | C10—C15 | 1.4002 (16) |
| N2—C4 | 1.4692 (13) | C11—C12 | 1.4017 (18) |
| C1—C2 | 1.5534 (13) | C11—H11A | 0.9500 |
| C2—C10 | 1.5362 (13) | C12—C13 | 1.372 (2) |
| C2—C16 | 1.5411 (14) | C12—H12A | 0.9500 |
| C2—C3 | 1.5509 (13) | C13—C14 | 1.372 (2) |
| C3—C4 | 1.5239 (15) | C13—H13A | 0.9500 |
| C3—H3A | 0.9900 | C14—C15 | 1.3918 (17) |
| C3—H3B | 0.9900 | C14—H14A | 0.9500 |
| C4—H4A | 0.9900 | C15—H15A | 0.9500 |
| C4—H4B | 0.9900 | C16—C21 | 1.3871 (17) |
| C5—C6 | 1.5147 (18) | C16—C17 | 1.3941 (16) |
| C5—H5A | 0.9900 | C17—C18 | 1.3832 (19) |
| C5—H5B | 0.9900 | C17—H17A | 0.9500 |
| C6—C7 | 1.518 (2) | C18—C19 | 1.375 (3) |
| C6—H6A | 0.9900 | C18—H18A | 0.9500 |
| C6—H6B | 0.9900 | C19—C20 | 1.380 (3) |
| C7—C8 | 1.507 (2) | C19—H19A | 0.9500 |
| C7—H7A | 0.9900 | C20—C21 | 1.390 (2) |
| C7—H7B | 0.9900 | C20—H20A | 0.9500 |
| C8—C9 | 1.522 (2) | C21—H21A | 0.9500 |
| C1—N1—H1NB | 121.7 (11) | C9—C8—H8A | 109.3 |
| C1—N1—H1NA | 121.3 (11) | C7—C8—H8B | 109.3 |
| H1NB—N1—H1NA | 116.7 (15) | C9—C8—H8B | 109.3 |

| | | | |
|--------------|-------------|-----------------|-------------|
| C5—N2—C9 | 109.79 (9) | H8A—C8—H8B | 107.9 |
| C5—N2—C4 | 110.75 (9) | N2—C9—C8 | 111.01 (12) |
| C9—N2—C4 | 110.90 (10) | N2—C9—H9A | 109.4 |
| O1—C1—N1 | 122.40 (10) | C8—C9—H9A | 109.4 |
| O1—C1—C2 | 122.01 (10) | N2—C9—H9B | 109.4 |
| N1—C1—C2 | 115.41 (9) | C8—C9—H9B | 109.4 |
| C10—C2—C16 | 109.30 (8) | H9A—C9—H9B | 108.0 |
| C10—C2—C3 | 105.96 (8) | C11—C10—C15 | 118.07 (10) |
| C16—C2—C3 | 112.46 (8) | C11—C10—C2 | 124.97 (10) |
| C10—C2—C1 | 114.55 (8) | C15—C10—C2 | 116.65 (10) |
| C16—C2—C1 | 103.17 (8) | C10—C11—C12 | 119.97 (12) |
| C3—C2—C1 | 111.55 (8) | C10—C11—H11A | 120.0 |
| C4—C3—C2 | 113.28 (8) | C12—C11—H11A | 120.0 |
| C4—C3—H3A | 108.9 | C13—C12—C11 | 121.18 (14) |
| C2—C3—H3A | 108.9 | C13—C12—H12A | 119.4 |
| C4—C3—H3B | 108.9 | C11—C12—H12A | 119.4 |
| C2—C3—H3B | 108.9 | C12—C13—C14 | 119.56 (12) |
| H3A—C3—H3B | 107.7 | C12—C13—H13A | 120.2 |
| N2—C4—C3 | 111.18 (8) | C14—C13—H13A | 120.2 |
| N2—C4—H4A | 109.4 | C13—C14—C15 | 119.87 (13) |
| C3—C4—H4A | 109.4 | C13—C14—H14A | 120.1 |
| N2—C4—H4B | 109.4 | C15—C14—H14A | 120.1 |
| C3—C4—H4B | 109.4 | C14—C15—C10 | 121.33 (12) |
| H4A—C4—H4B | 108.0 | C14—C15—H15A | 119.3 |
| N2—C5—C6 | 111.37 (11) | C10—C15—H15A | 119.3 |
| N2—C5—H5A | 109.4 | C21—C16—C17 | 118.48 (11) |
| C6—C5—H5A | 109.4 | C21—C16—C2 | 123.31 (10) |
| N2—C5—H5B | 109.4 | C17—C16—C2 | 118.18 (10) |
| C6—C5—H5B | 109.4 | C18—C17—C16 | 120.80 (14) |
| H5A—C5—H5B | 108.0 | C18—C17—H17A | 119.6 |
| C5—C6—C7 | 110.82 (12) | C16—C17—H17A | 119.6 |
| C5—C6—H6A | 109.5 | C19—C18—C17 | 120.31 (15) |
| C7—C6—H6A | 109.5 | C19—C18—H18A | 119.8 |
| C5—C6—H6B | 109.5 | C17—C18—H18A | 119.8 |
| C7—C6—H6B | 109.5 | C18—C19—C20 | 119.56 (14) |
| H6A—C6—H6B | 108.1 | C18—C19—H19A | 120.2 |
| C8—C7—C6 | 110.04 (12) | C20—C19—H19A | 120.2 |
| C8—C7—H7A | 109.7 | C19—C20—C21 | 120.52 (16) |
| C6—C7—H7A | 109.7 | C19—C20—H20A | 119.7 |
| C8—C7—H7B | 109.7 | C21—C20—H20A | 119.7 |
| C6—C7—H7B | 109.7 | C16—C21—C20 | 120.29 (13) |
| H7A—C7—H7B | 108.2 | C16—C21—H21A | 119.9 |
| C7—C8—C9 | 111.82 (13) | C20—C21—H21A | 119.9 |
| C7—C8—H8A | 109.3 | | |
| O1—C1—C2—C10 | −32.45 (15) | C3—C2—C10—C15 | −68.02 (12) |
| N1—C1—C2—C10 | 152.28 (10) | C1—C2—C10—C15 | 168.56 (10) |
| O1—C1—C2—C16 | 86.24 (13) | C15—C10—C11—C12 | 0.03 (17) |

| | | | |
|----------------|--------------|-----------------|--------------|
| N1—C1—C2—C16 | −89.03 (11) | C2—C10—C11—C12 | −173.31 (11) |
| O1—C1—C2—C3 | −152.81 (11) | C10—C11—C12—C13 | 1.2 (2) |
| N1—C1—C2—C3 | 31.92 (13) | C11—C12—C13—C14 | −1.6 (2) |
| C10—C2—C3—C4 | −65.67 (11) | C12—C13—C14—C15 | 0.8 (2) |
| C16—C2—C3—C4 | 174.97 (8) | C13—C14—C15—C10 | 0.40 (19) |
| C1—C2—C3—C4 | 59.61 (12) | C11—C10—C15—C14 | −0.80 (17) |
| C5—N2—C4—C3 | −82.56 (11) | C2—C10—C15—C14 | 173.09 (11) |
| C9—N2—C4—C3 | 155.28 (10) | C10—C2—C16—C21 | −133.26 (11) |
| C2—C3—C4—N2 | 167.45 (9) | C3—C2—C16—C21 | −15.87 (14) |
| C9—N2—C5—C6 | −60.68 (14) | C1—C2—C16—C21 | 104.46 (12) |
| C4—N2—C5—C6 | 176.51 (10) | C10—C2—C16—C17 | 48.96 (12) |
| N2—C5—C6—C7 | 57.66 (16) | C3—C2—C16—C17 | 166.35 (10) |
| C5—C6—C7—C8 | −52.61 (19) | C1—C2—C16—C17 | −73.32 (11) |
| C6—C7—C8—C9 | 52.17 (19) | C21—C16—C17—C18 | 1.61 (19) |
| C5—N2—C9—C8 | 59.41 (15) | C2—C16—C17—C18 | 179.50 (11) |
| C4—N2—C9—C8 | −177.87 (12) | C16—C17—C18—C19 | 0.0 (2) |
| C7—C8—C9—N2 | −56.18 (18) | C17—C18—C19—C20 | −1.1 (2) |
| C16—C2—C10—C11 | −133.19 (11) | C18—C19—C20—C21 | 0.4 (3) |
| C3—C2—C10—C11 | 105.40 (11) | C17—C16—C21—C20 | −2.26 (19) |
| C1—C2—C10—C11 | −18.01 (15) | C2—C16—C21—C20 | 179.98 (12) |
| C16—C2—C10—C15 | 53.39 (12) | C19—C20—C21—C16 | 1.3 (2) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N1—H1NB \cdots N2 ⁱ | 0.87 (1) | 2.08 (1) | 2.9457 (13) | 177 (2) |
| N1—H1NA \cdots O1 ⁱⁱ | 0.84 (1) | 2.38 (1) | 3.1971 (14) | 164 (2) |
| C3—H3B \cdots O1 ⁱⁱ | 0.99 | 2.47 | 3.3738 (14) | 152 |

Symmetry codes: (i) $-x+3/2, y, z+1/2$; (ii) $-x+3/2, y, z-1/2$.